

第 86 回「工学とバイオ」セミナー

(生産技術研究奨励会 RC-107 共催)

“Multi-scale Molecular Simulation of Biological Membranes:

~ Fighting the Corona Virus ~”

Prof. Florian Müller-Plathe (TU Darmstadt)

Date: March 10th (Tue) from 11AM-12AM

Place: C Lounge, IIS



Abstract:

The outer shell of corona viruses consists of a common biomaterial, a phospholipid membrane. Piercing the membrane is the key to the inactivation of the virus by disinfectants. During the Covid-19 pandemic, we used molecular simulation to study the mechanisms by which alcoholic disinfectants permeate the viral membrane and ultimately destroy it. More importantly, we also determined the minimum concentrations needed. An important side aspect is the use of simulation models of different levels of resolution and machine learning, which made these investigations possible.

References:

1. H. Eslami, S. Das, T. Zhou, and F. Müller-Plathe, *J. Phys. Chem. B* **124**, 10374-10385 (2020). [DOI: 10.1021/acs.jpcc.0c08296]
2. S. Das, M.K. Meinel, Z. Wu, and F. Müller-Plathe, *J. Chem. Phys.* **154**, 245101 (2021). [DOI: 10.1063/5.0055331]
3. T. Zhou, Z. Wu, S. Das, H. Eslami, and F. Müller-Plathe, *J. Chem. Theor. Comput.* **18**, 2597–2615 (2022). [DOI: 10.1021/acs.jctc.1c01120]

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